REPORT DOCUMENTATION PAGE

AFRL-SR-BL-TR-01-

0380

Public reporting burden for this collection of information is estimated to average 1 hour per response, inclu ... urces, gathering and maintaining the data needed, and completing and reviewing the collection of information. S ... of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Serv ... ferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Pap

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE	3. REP... ... AND DATES COVERED 01 SEP 1994 - 31 Aug 1997 Final

4. TITLE AND SUBTITLE
Growth and Characterization of CD 1-X ZNX TE on Silicon Substrate

5. FUNDING NUMBERS
63739E
B721/03

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR/NE
801 North Randolph Street Rm 732
Arlington, VA 22203-1977

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
F49620-94-C-0080

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION AVAILABILITY STATEMENT
APPROVAL FOR PUBLIC RELEASED; DISTRIBUTION UNLIMITED

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

Further optimize the growth parameters for CdTe on Si to improve the layer quality. Optimize conventional substrate preparation procedure and investigate new procedures. By studying the interface structure of CdTe/Si and strain relaxation in CdTe Layer. Study the interface structure by means of high resolution transmission electron microscopy and scanning transmission electron microscopy. Observe the surface morphology by optical microscopy.

20010625 164

14. SUBJECT TERMS

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

FINAL REPORT

For project supported by DARPA and monitored by AFFAIRS
(September 1, 1994 - August 31, 1997)

1. Contract Title: **GROWTH AND CHARACTERIZATION OF CdTe ON SILICON SUBSTRATES**

Number: F49620-94-C-0080

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Date: August 31, 1997

2. Technical Objectives:

To grow $Cd_{1-x}Zn_xTe$ of good quality on Si with the lattice constant matched to $Hg_xCd_{1-x}Te$, which will improve the quality of $Hg_xCd_{1-x}Te$ to be grown by LPE on $Cd_{1-x}Zn_xTe$.

Further optimize the growth parameters for CdTe on Si to improve the layer quality.
Optimize conventional substrate preparation procedure and investigate new procedures.
By studying the interface structure of CdTe/Si and strain relaxation in CdTe layer.
Study the interface structure by means of high resolution transmission electron microscopy and scanning transmission electron microscopy. Observe the surface morphology by optical microscopy.
Grow HgCdTe on CdTe/Si by both MBE and LPE

Grow CdTe(211)B on nominal Si(211).
Control the formation of twins and reduce threading dislocations at the interface.
Grow $Hg_{1-x}Cd_xTe$(211)B on CdTe(211)B/Si(211).
Understand interface formation of CdTe on Si.

3. Approaches:

- Growing CdTe on Si with various growth paramenters and substrate geometry
- Characterization of samples. Measuring the FWHM of x-ray double crystal rocking curve (DCRC) to determine the quality of the sample. Measuring the high-resolution electron microscopy to determine the interface quality. Observing the surface morphology by the optical microscopy.
- Correlation of growth parameters with sample quality as characterized.
- Growing $Cd_{1-x}Zn_{x}Te$ on Si by adding Zn atoms and taking advantage of the optimized growth condition for CdTe on Si.
- Determining the alloy composition by either x-ray diffractometer or spectroscopic ellipsometry.
- Correlating the Zn flux during the growth with the alloy composition
- Incorporation of the in-situ characterization tool to determine the alloy composition, which will aid in obtaining the desired alloy composition and homogeneity during growth
- Further optimize the growth parameters for CdTe on Si to improve the layer quality.
- Optimize conventional substrate preparation procedure and investigate new procedures.
- By studying the interface structure of CdTe/Si and strain relaxation in CdTe layer.
- Study the interface structure by means of high resolution transmission electron microscopy and scanning transmission electron microscopy. Observe the surface morphology by optical microscopy.
- Study the nucleation process of ZnTe buffer layer on Si(211).
  Grow $Hg_{1-x}Cd_{x}Te$ (211)B on CdTe(211)B/Si(211) by MBE and LPE.

4. Accomplishments:

I. The quality of CdTe grown on Si (001) substrate largely depends on the substrate geometry such as the off cut orientation angle θ relative to (001) and the azimuthal angle ϕ relative to (110). A number of samples were grown with various of-cut angles and azimuthal angles. Under the same growth condition the best quality was obtained with $\theta = 1°$ and $\phi \cong 30°$ as evidenced by the lowest value of the FWHM by x-ray rocking curve.

II. The quality of CdTe grown on the Si (001) substrate largely depends on the growth parameters such as initiation and thermal cycling annealing. Deoxidization of the substrate for the best surface was performed at various substrate temperature. The surface was also prepared with various precursors before growth. Different kinds of

thermal cyclic annealing was performed. In this way, the optimal growth condition was found.

III. Despite the large lattice mismatch between CdTe and Si, the best sample exhibited the FWHM of 60 arcsec.

IV. Under the optimum growth condition, twins were suppressed at the distances greater than 2.5 mm from the substrate surface.

V. ZnTe of high quality which is another binary and compound of Cd1-x Zn x Te was grown successfully.

VI. MPL has grown 135 CdTe and CdZnTe layers on Si substrates

VII. Comprehensive studies on the interface of CdTe/Si by TEM, STEM, XPS and RHEED indicate that the CdTe/Si interface is coherent over the large area. An interfacial layer probably SiTe2-type compound was found at the interface as a result of diffusion of Te atoms into the Si substrate. Such an interfacial layer absorbs most of the strains caused by the mismatch between the two materials so that CdTe layer can assume its natural lattice parameter almost at the interface.

VIII. Single domain and twin-free CdTe(111)B layers, with x-ray DCRC FWHM less than 100 arc sec, have been grown routinely on 40 tilted Si(001) substrates, which was optimized for LPE growth of HgCdTe, with good reproducibility.

IX. High quality CdTe (211)B layers, with mirror-like surface and x-ray FWHM less than 100 arc sec, have been grown on Si(211) substrates with good reproducibility.

X. The x-ray DCRC FWHM of the best 10 tilted CdTe(111)B, 40 tilted CdTe(111)B, CdTe(001) and CdTe(211)B layers are 60 arc sec, 75 arc sec, 58 arc sec and 74 arc sec, respectively.

XI. EPD of CdTe(211)B layers, evaluated by Texas Instruments, is as low as 2 ? 105 /cm2.

XII. HgCdTe layers have been grown on CdTe(111)B/Si(001) alternate substrates. The x-ray DCRC FWHM of as-grown HgCdTe layers are always lower than that of CdTe buffer layers. EPD of an annealed HgCdTe is 4.3 ? 106 /cm2. P-type Hg0.78Cd0.22Te exhibits a hole mobility of 432 cm2/Vs and lifetime of 70 ns at 80 K.

XIII. 30 CdTe(111)B/Si(001) layers have been delivered to Loral Infrared and Imaging Systems Inc. Single-domain and twin-free HgCdTe(111)B layers have been grown these alternate substrates by LPE. EPD of the HgCdTe layers is of the order of 5 ? 105 cm-2.

XIV. Photodiodes have been fabricated in Loral on HgCdTe layers LPE-grown on CdTe(111)B/Si(001) alternate substrates. The cut-off wavelength was estimated to be 9.5 ?m at 80 K. R0A value is 101 ohm.cm2

XV. MPL has established strong collaboration with several industrial partners, such as Loral Infrared and Imaging System, Rockwell Science Center and Texas Instruments. MPL is now in the process to establish a collaboration with Phillips Laboratory at Kirkland Air Force Base.

XVI. MPL has grown 172 CdTe, ZnTe and CdZnTe layers on Si substrates.

XVII. Systematic study on ZnTe nucleation process on Si indicate the possibility to control the orientation of CdTe on Si. Single domain, twins free CdTe(211)B and (133)B can be selectively grown on Si.

XVIII. Comprehensive studies on the microstructure reveal the formation of threading location and the lamella twins domains.

XIX. The low defect density of CdTe(211)B/Si has been confirmed by TEM. A thin ZnTe was demonstrated to help accommodate strains and block the propagation of dislocations.

XX. LWIR $Hg_{1-x}Cd_xTe(211)B$ layers have been grown by MBE on CdTe(211)B/Si(211) alternate substrates. *In situ* p-type and n-type doping has been performed successfully. The quality of $Hg_{1-x}Cd_xTe$ grown on CdTe/Si is comparable to that of layer grown on bulk CdTe(211)B.

XXI. DLPH p on n MWIR $Hg_{1-x}Cd_xTe(211)B/CdTe/Si$ photodiodes were fabricated at Rockwell Science Center. 77K quantum efficiency is about 61% for a cut-off wavelength of 5.3 μm without the antireflection coating layer. R_oA in the access of $1.6\times10^7\ \Omega cm^2$ at 77K.

XXII. Study on the CdTe(111)B/Si(001) microstructure by STEM provides more understanding on the nature of interface formation and growth mechanism.

XXIII. Strong collaborations between MPL and industrial companies have been continue. A new company EPIR ltd. has been started to supply the CdTe/Si substrates to the industrial.

7. Listing

During this contract, 8 regular contributed presentations and 21 journal papers have been given by MPL members.

a) Publications:

1. "Si 2p Core-Level at the CdTe/Si(100) Interface", R. Sporken, F. Malengreau, J. Ghijsen, R. Caudano, S. Sivananthan, J.P. Faurie, T. Von Gemmeren, and R.L. Johnson, Applied Surface Science (1997).

2. "High Quality Large Area CdTe(211)B on Si (211) grown by molecular beam epitaxy",S. Rujirawat, L.A. Almeida, Y.P. Chen, S. Sivananthan, David J. Smith, Appl. Phys. Lett, 71(13), 1810-1812, (1997).

3. "Temperature dependence of the optical properties of CdTe", C.C. Kim, M. Daraselia, J.W. Garland and S. Sivananthan, Phys. Rev. B. 56, 4786-4797 (1997).

4. "Atomic-scale observations of heteroepitaxial interfaces", David J. Smith, S. Sivananthan and S.-C. Y. Tsen, Interface Science and Materials Interconnection Proceedings, 92-98, (1997) .

5. "Optical investigation of strain and defects in (100) CdTe/Ge/Si and ZnTe/Ge/Si grown by molecular beam epitaxy", J.W. Hutchins, B.J. Skromme, Y.P. Chen, S. Sivananthan and J.B. Posthill, Appl. Phys. Lett. 71 (3), 350-352, (1997).

6. "Atomic layer graphoepitaxy for single crystal heterostructures", D.J. Wallis, N.D. Browning, S. Sivananthan, P.D. Nellist and S.J. Pennycook, Appl. Phys. Lett., 70 (23), 3113-5, (1997).

3. "HgCdTe(211)B grown on CdTe(211)B/ZnTe(211)B/Si(211) by MBE", S. Rujirawat, P.S. Wijewarnasuriya, L.A. Almeida, Y.P. Chen, F. Aqariden and S. Sivananthan, Mat. Res. Soc. Symp. Proc. 450, (1997).

4. " Growth and characterization of heteroepitaxial CdTe and ZnTe on Ge (001)buffer layers", David J. Smith, S.-C. Y. Tsen, J.B. Posthill, Y.P.Chen and S. Sivananthan, Appl. Phys. Lett. Sept. 1996

5. "Atomic layer graphoepitaxy for single crystal heterostructures, D.J. Wallis, N.D. Browning, S. Sivananthan, P.D. Nellist and S.J. Pennycook, Science, (submitted August,1996).

6. "Heteroepitaxial CdTe(111) grown by MBE on nominally flat and misoriented Si(001) substrates: characterized by electron microscopy and optical methods", S-CY Tsen, D.J. Smith, J. W. Hutchins, B. J. Skromme, Y.P.Chen, S. Sivananthan, J. of Cryst. Growth 159, 58-63(1996).

7. "Growth of high quality CdTe on Si substrates by molecular beam epitaxy", T. Almeida, Y.P. Chen, J.P. Faurie and S. Sivananthan, J. of Electron. Mater., Vol. 25, No. 8,1402-1405 (1996).

8. "Transient picosecond/subpicosecond Raman scattering studies of nonequilibrium electron distributions and phonons in CdTe", E. Grann, Y. Chen, K.T. Tsen, D.K. Ferry, T. Almeida, Y.P. Chen, and S. Sivananthan, J. Appl. Phys., Oct.

9. "Synchrotron x-ray photoconductor detector arrays made on MBE grown CdTe", S. S. Yoo, B.Rodricks, S. Sivananthan, J. P. Faurie, and P. A. Montano, J. of Electron. Mater. Vol. 25, 1306 (1996).

10. "Heteroepitaxy of II-VI semiconductors on silicon", R. Sporken, F. Malengreau, Y.P. Chen, T. van Gemmmeren, J.Ghijsen, and S. Sivananthan, Phyicalia Mag., May (1996)

11. "Heteroepitaxy of CdTe on Si substrates in view of infrared and x-ray detection", J.P.Faurie, A.Almeida, Y.P.Chen, R. Sporken and S. Sivananthan, 1996. SPIE Proceeding, Vol. 2658 (1996)

12. "Performance of MBE grown CdTe photoconductor arrays for hard x-ray detection ", S.S. Yoo, B.Rodricks, S.Sivananthan, J. P. Faurie, and P.A. Montano, J. of Cryst. Growth 159, 906-909(1996).

13. "Low temperature performance of an MBE grown CdTe x-ray photoconductor detector", Sung-Shik Yoo, B. G. Rodricks, S. Sivananthan, J. P. Faurie, and P. A. Montano, SPIE Proc. Vol. 2519, 87 (1995).

14. "New MBE CdTe photoconductor array detector for x-ray applications", S. S. Yoo, B.Rodricks, S. Sivananthan, J. P. Faurie, and P. A. Montano, Appl. Phys. Lett. 66(16) 2037 (1995).

15. "MBE Grown CdTe photoconductor array detector for x-ray measurements", S. S. Yoo, B. Rodricks, S. Sivananthan, J. P. Faurie, and P.A. Montano, Rev. Sci. Instr. 66(2), 2320 (1995).

16. "Microstructure of heteroepitaxial CdTe grown on misoriented Si(001) substrates", D.J. Smith, S.C.Tsen, Y.P. Chen, J.P. Faurie and S. Sivananthan, Appl. Phys. Lett. 67, 1591 (1995).

17. C. C. Kim and S. Sivananthan, "Modeling the Optical Dielectric Function of II-VI Compound CdTe," J. Appl. Phys. 78, 4003 (1995)

b) Presentations

1) "HgCdTe(211)B grown on CdTe(211)B/ZnTe(211)B/Si(211) by MBE", S. Rujirawat, P.S. Wijewarnasuriya, L.A. Almeida, Y.P. Chen, F. Aqariden and S. Sivananthan, 199Mat. Res. Soc. Symp. Proc. 450, (1997).

2) "Determination of the interface structure of CdTe(111) on Si(100), using Z-contrast imaging and EELS", D.J. Wallis, P.D. Nellist, S.Sivananthan, N.D. Browning and S.J. Pennycook, 54th Annual Meeting of the Microscopical Society of America, Minneapolis, August 11-15,1996

3) "Atomic Resolution EELS for composition and 3-D coordination determination at interfaces and defects", N.D. Browning, D.J. Wallis, S.Sivananthan, P.D. Nellist and S.J.

Pennycook, 54th Annual Meeting of the Microscopical Society of America, Minneapolis, August 11-15,1996

4) "Interface structure of CdTe/Si", N. D. Browning, C. H. Grein, J.P. Faurie, S. Rujirawat, T. Almeida, R. Sporken, D.J. Willis, S.-C. Y. Tsen, David Smith, and S. Sivananthan, Ninth International Conference on Molecular Beam Epitaxy, Malibu, CA, August 5-9, 1996.

5) "Current Status of CdTe on Si" (invited paper), S. Sivananthan, F. T. Smith, and W. P. Norton, IRIS Meeting, Colorado, July 29-30, 1996.

6) "Atomic-scale observations of heteroepitaxial interfaces" (invited paper), David J. Smith, S. Sivananthan and S.-C. Y. Tsen, 8th Japanese Inst. of Metals International Symposium, 1996

7) "Heteroepitaxy of CdTe on Si substrates in view of infrared and x-ray detection" (invited paper), J.P.Faurie, A.Almeida, Y.P.Chen, R. Sporken and S. Sivananthan, Phontonics West, San Jose, CA, Jan 27-Feb.2, 1996

8) "Orientation dependence of CdTe/Si grown by MBE," A.Almeida, Y.P. Chen, J.P.Faurie, Smith, Tsen, and S.Sivananthan, MRS Proceedings, Boston, MA November 28 1995

9) "Synchrotron -ray photoconductor detector arrays made on MBE Grown CdTe", S. S. Yoo, B. Rodricks, S. Sivananthan, J. P. Faurie, and P. A. Montano - The 1995 U. S. Workshop on Physics and Chemistry of Mercury Cadmium Telluride and Other IR Materials, Baltimore, MD, Oct. 10-12 1995

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